Describing the Absorption of Weak Electrolytes and Acid Gases with Ionic Liquids Using the Soft-SAFT Approach

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Ionic Liquids (ILs) are a family of compounds with a very wide variety of properties due to their particular physicochemical characteristics. In particular, their extremely low volatility marks them as environmentally benign alternatives to volatile organic solvents for separation processes. In this work, the solubility of three common pollutants; SO_2, NH_3 and H_2S, in ionic liquids (ILs) is studied using the soft-SAFT equation of state. New models guided by physical insight, based on statistical mechanics concepts, are proposed for these compounds. A relatively simple model is used for three different imidazolium ionic liquid families with different anions. The success of these simple models has been recently proved in mixtures of ILs with carbon dioxide, water and alcohols. A new set of molecular parameters for SO_2, NH_3 and H_2S is developed and very good agreement is shown for the phase envelope of those three compounds. Then, binary mixtures of these compounds with imidazolium-based ionic liquids are presented in an industrially relevant temperature range. Cross-association interactions have been considered under several assumptions based on previous experience and physical features. A single temperature independent energy binary parameter is sufficient to describe every family of mixtures in good agreement with the available data in the literature. In addition, a vapour-liquid-liquid equilibrium (VLLE) region has been identified for mixtures of hydrogen sulphide + imidazolium ionic liquids with the $[PF_6]^-$ anion at higher H_2S. These simple models allow an accurate description of the phase absorption diagrams of those complex mixtures.

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